Urea, 1-(2-chloroethyl)-3-(2,2,2-trifluoroethyl)-

Inchi: InChI=1S/C5H8ClF3N2O/c6-1-2-10-4(12)11-3-5(7,8)9/h1-3H2,(H2,10,11,12)
InchiKey: BXZXTELFZRVLKU-UHFFFAOYSA-N
Formula: C5H8ClF3N2O
SMILES: OC(=NCCCl)NCC(F)(F)F
Mol. weight [g/mol]: 204.58
CAS: 13908-00-4

Physical Properties

Property code	Value	Unit	Source
hf	-785.68	kJ/mol	Joback Method
hvap	53.87	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	1.291		Crippen Method
mcvol	120.390	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
tb	564.72	K	Joback Method
tc	741.28	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908004&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature